

Tunable Superfluidity and Quantum Magnetism with Ultracold Polar Molecules

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(Received 9 June 2011; published 8 September 2011)

By selecting two dressed rotational states of ultracold polar molecules in an optical lattice, we obtain a highly tunable generalization of the t - J model, which we refer to as the t - J - V - W model. In addition to XXZ spin exchange, the model features density-density interactions and density-spin interactions; all interactions are dipolar. We show that full control of all interaction parameters in both magnitude and sign can be achieved independently of each other and of the tunneling. As a first step towards demonstrating the potential of the system, we apply the density matrix renormalization group method to obtain the 1D phase diagram of the simplest experimentally realizable case. Specifically, we show that the tunability and the long-range nature of the interactions in the t - J - V - W model enable enhanced superfluidity. Finally, we show that Bloch oscillations in a tilted lattice can be used to probe the phase diagram experimentally.

DOI: 10.1103/PhysRevLett.107.115301

PACS numbers: 67.85.-d, 33.80.-b, 71.10.Fd, 71.10.Pm

Experiments with ultracold atoms have recently extended the range of candidate systems for realizing unconventional states of matter and enabled the simulation of models describing condensed matter phenomena [1]. One major goal of current research at this interface between condensed matter and atomic physics is to emulate the Heisenberg and t - J models, which are believed to underlie certain quantum magnetic materials [2] and high-temperature superconductors [3], respectively. However, in the ultracold atom realization of these models, the small superexchange interaction J [1] makes the underlying physics extremely challenging to observe. At the same time, ultracold polar molecules [4], such as KRb [5,6] and LiCs [7], have recently been produced in their electronic and rovibrational ground states. In this Letter, we show that when such molecules are localized in an optical lattice, their rotational degree of freedom can be used to simulate tunable Heisenberg-like models at unit filling of the lattice and, in the presence of doping, a fully tunable generalization of the t - J model that we refer to as the anisotropic t - J - V - W model. Dipole-dipole interactions that give rise to this model are orders of magnitude stronger than superexchange interactions J in ultracold atoms and can therefore better compete with other relevant energy and time scales such as, for example, those responsible for decoherence. Moreover, we show that the resulting long-range interactions are fully controllable with dc electric and continuous-wave microwave fields. As a first step towards demonstrating the potential of the model, we use the density matrix renormalization group method [8] to obtain the 1D phase diagram for the simplest experimentally relevant case and show that, at low fillings, the superfluid phase is enhanced relative to the

one in the conventional t - J model [9]. We propose to probe the phase diagram by using center-of-mass Bloch oscillations. Given that KRb has already been loaded into a 3D lattice, our proposal is applicable to current experiments.

The Hamiltonian and its features.—We consider diatomic polar molecules in their electronic and vibrational ground state partially polarized by a dc electric field along \hat{z} , confined to the x - y plane [10], and loaded in that plane into the lowest band of a square optical lattice. As described below, microwave fields are used to isolate in each molecule two dressed rotational states $|m_0\rangle$ and $|m_1\rangle$ and to obtain the t - J - V - W Hamiltonian

$$H = -t \sum_{\langle i,j \rangle m} [c_{im}^\dagger c_{jm} + \text{H.c.}] + \sum_{i \neq j} |\mathbf{R}_i - \mathbf{R}_j|^{-3} \times \left[\frac{J_\perp}{2} S_i^+ S_j^- + \frac{J_z}{2} S_i^z S_j^z + \frac{V}{2} n_i n_j + W n_i S_j^z \right]. \quad (1)$$

The two terms describe tunneling and dipole-dipole interactions, respectively; $\langle \rangle$ denotes nearest-neighbor bonds. Specifically, c_{jm}^\dagger creates a fermionic [5] or bosonic [6,7] molecule on site j (position \mathbf{R}_j) in dressed rotor state $m \in \{m_0, m_1\}$; in this Letter, we focus on fermions. Large reaction rates [10] between two molecules on the same site enforce the hard-core constraint. We define $n_{jm} = c_{jm}^\dagger c_{jm}$, $n_j = \sum_m n_{jm}$, $S_j^+ = c_{jm_0}^\dagger c_{jm_1}$, and $S_j^z = (n_{jm_0} - n_{jm_1})/2$ and use units in which $\hbar = 1$. The J_z , V , and W terms can be understood by thinking of $|m_0\rangle$ and $|m_1\rangle$ as classical permanent dipoles oriented along \hat{z} , while the $|m_0\rangle - |m_1\rangle$ transition dipole moment gives rise to the J_\perp term. We tune these dipole moments by constructing

Report Documentation Page				Form Approved OMB No. 0704-0188	
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1. REPORT DATE JUN 2011		2. REPORT TYPE		3. DATES COVERED 00-00-2011 to 00-00-2011	
4. TITLE AND SUBTITLE Tunable Superfluidity and Quantum Magnetism with Ultracold Polar Molecules				5a. CONTRACT NUMBER	
				5b. GRANT NUMBER	
				5c. PROGRAM ELEMENT NUMBER	
6. AUTHOR(S)				5d. PROJECT NUMBER	
				5e. TASK NUMBER	
				5f. WORK UNIT NUMBER	
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) California Institute of Technology, Institute for Quantum Information, Pasadena, CA, 91125				8. PERFORMING ORGANIZATION REPORT NUMBER	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)				10. SPONSOR/MONITOR'S ACRONYM(S)	
				11. SPONSOR/MONITOR'S REPORT NUMBER(S)	
12. DISTRIBUTION/AVAILABILITY STATEMENT Approved for public release; distribution unlimited					
13. SUPPLEMENTARY NOTES					
14. ABSTRACT					
15. SUBJECT TERMS					
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT Same as Report (SAR)	18. NUMBER OF PAGES 5	19a. NAME OF RESPONSIBLE PERSON
a. REPORT unclassified	b. ABSTRACT unclassified	c. THIS PAGE unclassified			

W , J_z , and J_\perp [31]. We find that in a small sphere in the four-dimensional $(dE/B, a, b, c)$ space around the point $(dE/B, a, b, c) = (2.97, 0.059, 0.56, 0.38)$, where $J_z = J_\perp = V = W = 0$, one can achieve any value of V , W , J_z , and J_\perp up to an overall positive prefactor. Similarly, in the special case where a single microwave couples $|\bar{1}\rangle$ and $|1\rangle$, we have a two-dimensional $(dE/B, b)$ subspace (with $a = 0$, $c = 1 - b$), in which J_z and J_\perp can be fully controlled—for simulations of the XXZ model at unit filling—around $(dE/B, b) = (4.36, 0.56)$, where they both vanish. While these examples prove full controllability in their respective cases, for any desired relationship between V , W , J_z , and J_\perp , there is likely a different level configuration that gives stronger interactions and uses weaker E , lower microwave intensity, and/or more convenient microwave frequencies.

Phase diagrams of the nearest-neighbor and dipolar t - J_\perp chains.—The full tunability of the t - J - V - W model provides access to a great variety of models with potentially exotic physics. As the simplest example of this physics, we present in Fig. 2 the 1D phase diagram in the limit $V = W = J_z = 0$, which is one of the simplest experimentally achievable cases (see above). Before analyzing dipolar interactions, we present in Fig. 2(a) the phase diagram of the nearest-neighbor t - J_\perp chain as obtained by

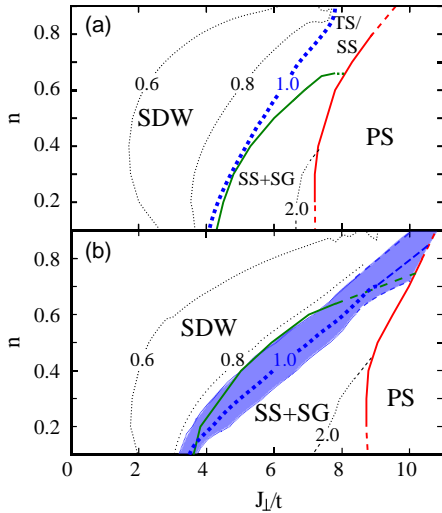


FIG. 2 (color online). Phase diagrams of the t - J_\perp chain with (a) nearest-neighbor and (b) dipolar J_\perp . We identify a metallic (repulsive Luttinger liquid) phase with dominant spin-density-wave correlations (SDW), a gapless superfluid with dominant triplet and singlet superfluid correlations (TS/SS), a singlet superfluid with a spin gap (SS + SG), and phase separation (PS). The spin gap is $\approx 0.35t$ in (a) and $\approx 0.7t$ in (b). Solid lines indicate phase transitions (green, SG closes; red, inverse compressibility becomes zero); dashed lines are extrapolations. The numbers show the value of K_ρ on the dotted lines. The line $K_\rho = 2$ is a crossover line within the SS + SG phase [32]. The shaded region in (b) displays $K_\rho = 1 \pm 0.15$ as an estimate of the numerical accuracy.

using the density matrix renormalization group method and following the analysis of Ref. [9]. The diagram is qualitatively similar to that of the standard t - J chain [9]: At fillings $n < 0.65$, we identify a repulsive Luttinger liquid (Luttinger parameter $K_\rho < 1$) with dominant spin-density-wave (SDW) correlations, an attractive Luttinger liquid ($K_\rho > 1$) with dominant singlet and triplet superfluid correlations, a singlet superfluid with a spin gap, and phase separation. At larger fillings, the spin gap is always zero, but the other phases remain.

In Fig. 2(b), we present the phase diagram of this system in the presence of dipolar interactions. At low fillings, SDW, the gapped singlet superfluid, and phase separation are obtained. This suggests that experiments with ultracold molecules can be a useful tool for exploring the phase diagram of the standard t - J model for arbitrary values of J in contrast to $J \ll t$ in ultracold atom realizations. At the same time, crucially, both diagrams in Fig. 2 feature a significant enhancement of the superfluid region compared to the original t - J model because the absence of attractive density-density interactions suppresses phase separation. Furthermore, the maximum value of the spin gap in the dipolar t - J_\perp chain ($\sim 0.7t$) is twice that in the nearest-neighbor t - J_\perp chain ($\sim 0.35t$), which is, in turn, twice that in the original t - J model. The larger spin gap should facilitate its experimental observation. Note that, as a conservative estimate of the numerical errors in computing K_ρ in the presence of long-range interactions with up to 100 sites, we estimate the true line $K_\rho = 1$ to lie in the shaded region $0.85 \leq K_\rho \leq 1.15$. Thus, the gapless superfluid cannot be identified in Fig. 2(b) within our numerical precision. Furthermore, while the line $K_\rho = 1$ and the line where the spin gap closes may coincide, our analysis of the correlation functions cannot rule out the existence of an exotic intermediate phase with a spin gap, $K_\rho < 1$, and dominant superfluid correlations.

Preparation and detection.—Ground states at specific points in the phase diagram can be prepared, e.g., by applying an additional microwave field coupling $|m_0\rangle$ and $|m_1\rangle$ and performing an adiabatic passage from an easily accessible state to the desired ground state by tuning the Rabi frequency and the detuning of the microwave field [18]. Direct probing of molecules [33] and conversion of molecules back to atoms [5] can in principle both be used for detection via noise correlations in the time of flight [1] or via *in situ* single-site imaging [34,35].

As a specific example of a detection technique available in current experiments, we propose to use Bloch oscillations [36,37]. In Fig. 3, we present our results as obtained via the Krylov-space variant of the adaptive time-dependent density matrix renormalization group method [38,39] for 20 sites when adding a linear field along the chain at filling $n = 0.1$ and $n = 0.2$ for different values of J_\perp/t . In the singlet superfluid, the amplitude of the oscillations drops and the frequency of the oscillations doubles

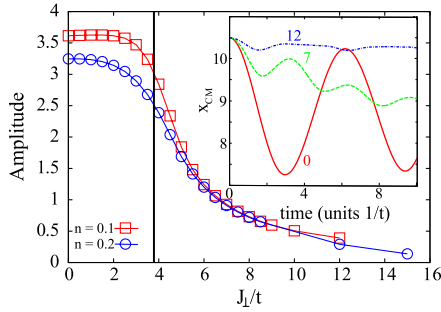


FIG. 3 (color online). Bloch oscillations in a dipolar t - J_{\perp} chain of 20 sites with open boundary conditions at fillings $n = 0.1$ and 0.2 , and tilting field $E_{\text{tilt}}/t = 1$ per site. The main plot shows the difference between the center-of-mass position x_{CM} at time zero and at the first minimum. The vertical line indicates the approximate value of J_{\perp}/t , at which the spin gap closes for $n = 0.2$. The inset shows the time evolution of x_{CM} at $n = 0.2$ at three indicated values of J_{\perp}/t .

(see $J_{\perp}/t = 7$ in the inset) relative to the gapless phase due to the presence of bound pairs. Bloch oscillations should be observable in direct absorption imaging [33]. While neither the frequency nor the amplitude of the oscillations show any sharp features at this small system size, the fit of experimental data to numerical results should allow for the location of the phase transition (vertical line in Fig. 3) even for small system sizes. As a complementary method for identifying the transition, we propose spectroscopic measurement of the spin gap [40].

Outlook.—We have presented a toolbox for simulating a highly tunable anisotropic t - J - V - W model with polar molecules. The advantages of this molecular toolbox over its atomic counterpart are higher energy scales and independent tunability of interactions and tunneling. This toolbox should enable the simulation of condensed matter phenomena, as well as the stabilization and controllable preparation of unconventional phases, such as d -wave superfluids [3]. The phase diagram of the experimentally simple case of a t - J_{\perp} chain shows an enhanced superfluid region, which we propose to probe via Bloch oscillations. We expect that the 2D t - J - V - W model can similarly be tuned into exhibiting enhanced superfluidity [41].

The present Letter also opens other exciting research avenues. In particular, natural extensions of the model include [30] spatially anisotropic interactions produced by a tilt in the dc electric field, spin-dependent tunneling obtained by adjusting lattice beams, $S > 1/2$ models realized by choosing more than two dressed states, and systems with an orbital degree of freedom encoded in the nuclear spin. Moreover, by considering molecular Wigner crystals [25,42,43], where the intermolecular distances are smaller than in an optical lattice, one can further increase the interaction strength. Furthermore, by analogy with Ref. [18], we expect our ideas to be extendable to

Rydberg atoms. Finally, one can envision applications of the present system to quantum computation (especially if one uses nuclear spin to store information), precision measurements, and controlled quantum chemistry [4].

We thank A. Muramatsu, M. Troyer, A. Moreno, D. Jin, G. Refael, J. Aldegunde, P. Julienne, M. Babadi, I. Bloch, P. Rabl, G. Quémener, A. Potter, B. Wunsch, P. Zoller, S. Pielawa, E. Berg, A. Daley, F. Mila, R. Noack, and H. Weimer for discussions. This work was supported by the NSF, NIST, the Lee A. DuBridge Foundation, the ARO with funding from DARPA-OLE, CUA, and AFOSR MURI. We acknowledge CPU time at ARSC.

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